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TIGHTENING (COMPACTION) OF BI-COMPONENT MICROMECHANICAL (GRANULAR) SYSTEM

Introduction. *One of the traditionally relevant problems of the theoretical framework for production and technology is the description, parameterization, and prediction of the properties of the mix depending on the parameters of the mix components. One of the most significant problems that hinder the effective use of granular materials, for example, in the construction industry, is the difficulty of ensuring their maximum compaction to increase the efficiency of their practical application.*

Problem Statement. *The understanding of the principles due to which the basic parameters of such systems are formed is based on theoretical models that allow the parameterization of the measurement data in terms of parameters that characterize the individual pure components (reference data). The construction of such models is a very difficult task that requires phenomenological information from alternative sources.*

Purpose. *Based on the Kirkwood-Buff theory and the data of analysis of experimental data on the study of macroscopic parameters of bi-dispersed granular mix we have developed a theoretical algorithm for describing and parameterizing its physical and mechanical characteristics in terms of its macroscopic and partial properties.*

Materials and Methods. *The methods of theoretical statistical physics for bi-component model systems, in particular the Kirkwood-Buff theory, the model equation of the state (the Carnahan-Starling equation), and phenomenological information on the dynamics of compaction of binary granular mixes have been used in the research.*

Results. *Using the Kirkwood-Buff and Carnahan-Starling theories and phenomenological data, we have developed a continuous description of the macroscopic properties of binary granular systems, which operates on the partial parameters of its components.*

Conclusions. *The obtained data have confirmed the influence of multi-dispersion on the dynamics of compaction, i.e. the mix ability to change its local structure of packing under external impact.*

Keywords: granular screen technologies, granular bi-component mix, Kirkwood-Buff theory, packing, compaction, Carnahan-Starling model, liquid mixes, and excess properties of mixes.

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The use of materials in the granular (micro-mechanical) state is typical for many industries and technologies. For example, granular materials have a lion's share in the products that are produced, consumed or used at certain stages of construction, light, food, mining, chemical, pharmaceutical, metallurgical and other industries. The variety of applications of such materials requires the ability to reliably parameterize their macroscopic properties, given the external effects that arise in the course of manipulations with them. The relationship between the macroscopic properties of the granular material (for example, ordering in the form of crystallization) and its macroscopic parameters, which purely determines its ability to maintain normal conditions and to provide the necessary effects (to stop or to transmit radiation of various types, to resist load due to the arch (bridging) effect, or to prevent aggregation in the course of stirring) also plays an important role. One of the examples of a significant need for algorithms of targeted manipulation of macroscopic parameters by external influences is structures that use protective modules containing granular substance. Such «granular screens» may potentially perform their regular functions quite reliably and, at the same time, have obvious advantages over the monolithic systems. So, in particular, they are:

a) not subject to radiation embrittlement;
b) easy to manipulate;
c) compactable and loosenable;
d) easy to replace and to transport;
e) efficient (in terms of production and operation).

In general, the mix problems take a prominent place in the engineering models for predicting the state of environment. For example, research [1] deals with predicting the sediment transport and river morphodynamics, which is a complicated problem for the rivers with a gravel bed, where the sediment mixes have different particle sizes. The authors have shown that the problem of binary packing is important for the correct estimation of the porosity of the gravel layer. In practice, it can be combined with calculations of dynamic models of sediment transport to predict morphodynamics in the rivers with gravel bed.

The theoretical models of granular materials that allow describing and predicting their properties have been developed in detail for the cases of specific conditions of their creation and use, in particular, the dimension, density of packing, and the nature of external influences. Unfortunately, there has been still no universal theory of granular materials, which takes into consideration all the observed properties. However, in many specific cases, it is possible to offer more or less adequate models of the description of the observed properties.

Materials used, for example, in nuclear reactors, are exposed to intense fluxes of ionizing radiation, mainly fast neutrons that are products of fission of nuclear fuel. Neutrons, while interacting with matter, transfer their energy to atoms through elastic collisions and also act as a source of the formation of fast charged particles (electrons, protons, and α-particles). The ultimate result of these processes is the destruction of the ordered arrangement of atoms in the crystal lattice of metal and the formation of foreign atoms, such as helium and hydrogen. The changes in the material structure, which are caused by radioactive effects, are called radiation damage [2].

A characteristic phenomenon that can accompany radiation damage to the material is shifting atoms from the crystal lattice sites and forming point defects, vacancies and interstitial atoms. A typical feature of fast neutron irradiation is the occurrence of cascades of atomic collisions in the irradiated material, which lead to the formation of microscopic areas of structural damage with a high concentration of point defects. Under the influence of temperature, the initial state of damage undergoes transformations, as a result of thermally activated migration of point defects, which is accompanied by their mutual recombination, annihilation in flight, and formation or dissociation of clusters.

In the radiation industry, the brittle fracture of metals is known to practically occur upon reac-

hing a strength criterion of 500—600 MPa. It has been found [2] that the irradiated metal contains stress concentrators in the form of brittle cracks that may be caused by plastic deformation as well.

It is clear that in the granular materials of any degree of packing, such processes occur according to completely different scenarios. These materials are already completely brittle. Therefore, the use of micromechanical systems as protective modules that are in direct contact with radiation is an attractive innovative idea [3]. Of course, the most effective will be a material in which the maximum compaction can be achieved along with the disorder, in a relatively simple way.

In the proposed research, we focus on the means of achieving the maximum compaction in a bi-component granular system, both in absolute value and in the rate of reach of such a state.

The study of the physical properties of simple bi-component mixes with the use of the methods of statistical mechanics is one of the traditionally relevant and very complicated problems of statistical physics of solutions. A well-known statistically substantiated theoretical approach in this field is the Kirkwood-Buff (KB) approach [4] that allows us to write down the basic thermodynamic quantities in terms of correlation integrals. The granular mixes (for example, bi-component ones) are known to have different degrees of packing, depending on the asymmetry (the ratio of molar fractions and the size of their components). Although the limiting fraction of packing can be parameterized with the use of only geometric considerations (the Voronoi-Delaunay method), the dynamics of granules in conglomerations that are under the influence of external small shocks remain a rather complex multi-parametric process. The Voronoi method of geometric constructions due to its purely geometric nature allows describing the structure of a fairly wide class of systems. To construct them for a given set of points, it is necessary to allocate a space around each point of the system, in which there are all the points that are closest to it, with the translation of this condition to the other points of the system. Thus, each point (the coordinate of which is determined by the position of the center of mass of the granular particle) is associated with its own characteristic volume (or area). Moreover, the volumes of the configurations are additive and completely cover the volume of the system. This is an important feature for the application of the approach in the case of granular mixes. It should be noted that the nature of the interaction between the particles does not directly affect the dividing procedure [5]. Experimental studies of granular mixes allow the obtainment of information about the distribution of particle centers at a certain time and, thus, the parameterization of the structure with the use of the Voronoi method. The study of the structure with the help of Voronoi's geometric constructions is based on the analytical analysis of the distribution of the areas of all system particles. Obviously, this approach enables obtaining information not only about the order (symmetry) or disorder of the system, but also about the distribution of free volume and its changes caused by external perturbations. Free volume is the main parameter that controls the behavior of granular mixes. It has been experimentally observed that the characteristic compaction time may differ when the ratio of the component particle size approaches a certain critical value. The mobility of the granules in the pack is the lowest in the vicinity of the penetration threshold (when small particles can still pass through void space between the large ones). Also, acceleration in the dynamics of compaction at sufficiently large ratio of the component sizes has been reported [6].

The problem of determining the maximum number of solid identical spherical particles (granules) can fill a given volume (a given shape) is among the traditional mathematical problems [7—11]. The characteristic parameter that determines the degree of packing η is, as a rule, the volume of all particles divided by the observed volume. It is assumed that its maximum value corresponds to face-centered symmetry (*fcc*), $\eta_{fcc} = \pi/\sqrt{18} = 0.74$ with disordered (frozen) packing (*rcp*) that corresponds to $\eta_{rcp} = 0.64$ as well as disordered loose

packing (*rlp*) that characterizes the mechanically stable configuration in the Earth's gravitational field $\eta_{rlp} = 0.60$ [12—14] as additional typical packing scale factors. Under the conditions of reduced gravity (micro-gravity), according to some data [8, 14, and 15], η may decrease to $\eta_{rlp} = 0.55$. It should be noted that the relationship between η and the nature (symmetry) of the granule location in the packed structure has been insufficiently studied so far [8,14].

If the degree of packing exceeds η_{rcp}, there are effects of ordering (symmetry) of the system. In particular, in [16—18], it has been reported that the crystallization phenomenon in the packing of solid spheres is observed (provided certain conditions are met). In 2D solid disk systems, crystallization is observed in the compaction path, i.e. under the conditions of gentle shaking of the system [16]. In many research works, crystallization is recognized as a driver for the processes of granular compaction, and the crystalline phase growth laws quite satisfactorily describe the patterns of compaction observed. The 3D problem is usually more complicated and, at the same time, closer to practical applications. Some research works are based on assumption of the scenario in which tetrahedral structures appear as growth nuclei of dense regions [18]. Also it should be mentioned that crystallization can be obtained by putting the system in an external field of vibration accelerations [19, 20], or by perturbations such as cyclic shift [21].

Given the data showing that the granular mixes are packed much denser than the monodisperse ones (consisting of the same, in the simplest case, spherical granules), considering the dependence of the parameters of such processes on the composition and particle size is very relevant. In this way, both direct physical [22] and numerical [23—25] studies have been conducted. Thus, in [26], a granular mix consisting of grains of different sizes has been studied numerically. The authors have concluded that the ratio of size and molar concentrations of the mix components are the main parameters that determine the formation of the current and the maximum achievable fractions of packing. Moreover, due to the fact that the vibration of groups of particles is a property that is reliably available for parameterization only in numerical simulations, it is the factor that actually prevents the observation of changes in the mix parameters. Sometimes (see [27]), such difficulties are not discussed by the authors and therefore the role of the above factor remains unclear.

As proposed in [28], we can consider the two threshold cases for binary mixes made of small and large balls. In the first case, the share of large (-sized) particles is high, so they form a system where the small particles occupy the remaining voids. When the particle size ratio is large enough, the small particles can get through the voids around the large ones. Conversely, when the share of small particles increases, the large particles are isolated in the environment of the small ones. In the first case, the system can be conditionally classified as "gravel" while, in the second case, it can be considered "pudding". It is clear that both extreme cases lead to different degrees of packing. However, the theoretical description of such extreme cases is usually made separately from each other. No single approach containing both the above threshold cases has yet existed. Our research deals with developing such an approach. In this way, we propose to use the ratio of statistical physics, despite the dissipative nature of the studied systems. Almost all of them have many quasi-stationary states in which they can be considered satisfying the criteria for using the apparatus of statistical mechanics to determine their macroscopic properties [29, 30].

The presentation of the main material

The classical Kirkwood-Buff formula for a bi-component mixture has the form [31]:

$$\beta_T^{(12)} = \frac{1}{k_B T} \cdot \frac{1 + n_1 G_{11} + n_2 G_{22} + n_1 n_2 (G_{11} G_{22} - G_{12}^2)}{n_1 + n_2 + n_1 n_2 (G_{11} + G_{22} - 2G_{12})}, \quad (1)$$

where $\beta_T^{(12)}$ is isothermal compressibility of a mix whose components are numbered 1 and 2; $n_1 = N_1/V$

and $n_2 = N_2/V$ are partial number densities of the particles, respectively; G_{11}, G_{22}, and G_{12} are the so called correlation integrals; k_BT is energy scale.

Correlation integrals $G_{\alpha\beta}$ are related with partial structural factors $S_{\alpha\beta}(0)$ by the following relationship:

$$S_{\alpha\beta}(0) = x_\alpha \delta_{\alpha\beta} + x_\alpha x_\beta n_{12} G_{\alpha\beta}, \quad (2)$$

where x_α, x_β are molar fractions of the mix components; $\delta_{\alpha\beta}$ is the Kronecker symbol; $n_{12} = N/V = (N_1 + N_2)/V = n_1 + n_2$ are number densities of particles for the mix.

Using formula (2) one may obtain:

$$S_{11}(0) = (1 - x) + (1 - x)^2 n_{12} G_{11}, \quad (3)$$

$$S_{22}(0) = x + x^2 n_{12} G_{22}, \quad (4)$$

$$S_{12}(0) = x(1 - x) n_{12} G_{12}, \quad (5)$$

where x is molar fraction of the 2nd component of the mix.

Having substituted the relationships (3)–(5) into the Kirkwood-Buff formula (1), we find the relationship between the isothermal compressibility of the bi-component mix and the partial structural factors in the following form:

$$\beta_T^{(12)} = \frac{1}{n_{12} k_B T} \cdot \frac{S_{11}(0)\, S_{22}(0) - S_{12}^2(0)}{x^2 S_{11}(0) - 2x(1 - x)\, S_{12}(0) + (1 - x)^2 S_{22}(0)}. \quad (6)$$

Given the fact that the structural factor of monodisperse system is defined as:

$$S(0) = 1 + nG = n k_B T \beta_T, \quad (7)$$

and given (3) and (4), we find that the expressions for partial structural factors of monodisperse phases $S_{11}(0)$ and $S_{22}(0)$ with partial isothermal compressibilities $\beta_T^{(1)}$ and $\beta_T^{(2)}$:

$$S_{11}(0) = (1 - x) \cdot n_1 k_B T \beta_T^{(1)}, \quad (8)$$

$$S_{22}(0) = x \cdot n_2 k_B T \beta_T^{(2)}. \quad (9)$$

Partial isothermal compressibilities $\beta_T^{(1)}$ and $\beta_T^{(2)}$ may be determined with the use of model equations of state. For example, using the Carnahan-Starling equation, we obtain the following expression for compressibility [32]:

$$\beta_T^{(i)} = \frac{1}{n_i k_B T} \cdot \frac{(1 - \eta_i)^4}{1 + 4\eta_i + 4\eta_i^2 - 4\eta_i^3 + 4\eta_i^4}, \quad i = 1; 2, \quad (10)$$

where $\eta_i = \frac{1}{6}\pi \sigma_i^3 n_i$ is the partial parameter that describes the degree of compaction of the i-th mix component.

Using the data on the mix isothermal compressibility $\beta_T^{(12)}$ obtained from alternative sources, for example, from an experiment, or by numerical simulation, having solved (6) with respect to the structural factor $S_{12}(0)$ we obtain:

$$S_{12}(0) = x(1 - x) f_{12} \pm \frac{\pm \sqrt{x^2 (1 - x)^2 f_{12} + S_{11} S_{22} - f_{12} \{x^2 S_{11} + (1 - x)^2 S_{22}\}}}{}, \quad (11)$$

where $f_{12} = n_{12} k_B T \beta_T^{(12)}$ is the value that can be determined with the help of the equation of spherical particle binary mix state [33], by the formula:

$$\beta_T^{(12)} = \frac{1}{n_{12} k_B T} \cdot \frac{(1 - \eta)^4}{1 + a\eta + b\eta^2 + c\eta^3 + d\eta^4}, \quad (12)$$

where a, b, c, d depend (in a known way) on x (або $f = \eta_2/\eta$), and on $\alpha = \sigma_1/\sigma_2$ (where σ_1 and σ_2 are diameters of the 1st and the 2nd components of the mix, respectively). Also, here we present the following useful relationships:

$$f = \frac{x}{\alpha^3 - (\alpha^3 - 1) \cdot x}, \; x = \frac{\alpha^3 \cdot f}{1 + (\alpha^3 - 1) \cdot f}. \quad (13)$$

In [6], experimental data have been obtained for compacting a binary mix of spherical particles with different degrees of size differences $\alpha = 2 \div 35$. The obtained data have been parameterized in the two characteristic threshold states of the mix. In the one state, the content of large particles prevails (the gravel case), whereas in the other one, the small particles are prevalent (the pudding case). In [34], an attempt has been made to describe the obtained experimental data in all intermediate states using weight functions that play the role of fitting parameters and, strictly speaking, tending towards the same threshold states. Thus, despite the previous results, the theoretical description of the macroscopic properties (including com-

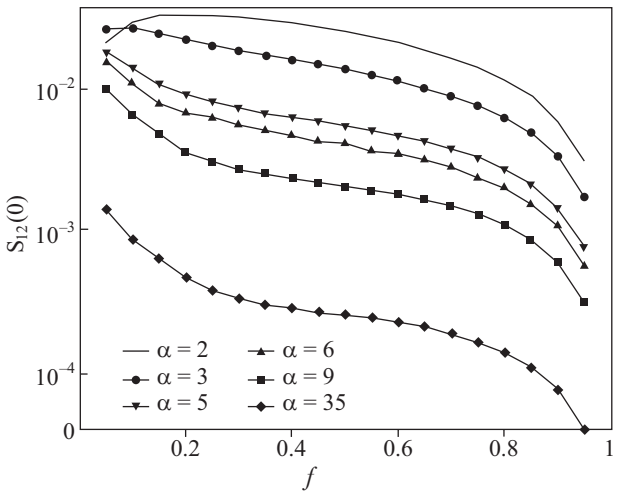

Fig. 1. The value of the partial structural factor $S_{12}(0)$ of the binary mix, depending on the volume fraction of the small component (f), calculated by formula (11) with the use of experimental data obtained in [6]. The difference in particle size of the mix components varies parametrically within $\alpha = 2 \div 35$

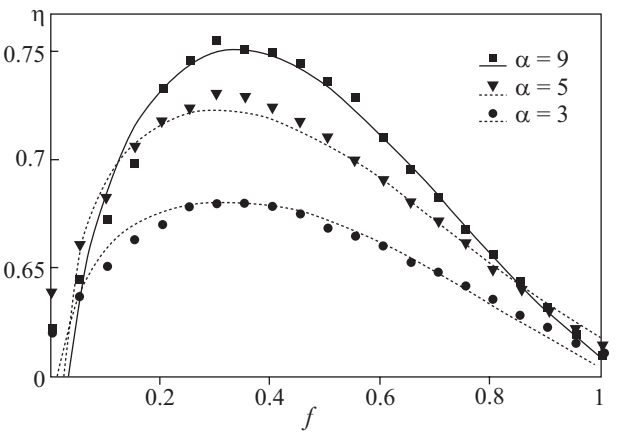

Fig. 2. The mix packing parameter (η) as function of (f): (-) – is theoretical approximation within the framework of the constructed theoretical approach; (o) is experimental data [6]

paction) of a binary mix within a single theory still remains an urgent task.

In our proposed research we have developed a single approach to the description of mix compaction using elements of statistical theory of mixes and model equations of state. The obtained results have been compared with the data of direct experimental measurements in [6].

Given formulas (3)—(4), (8) — (10), and (12), let us find first S_{12} (formula (11)). Figure 1 shows the results of the corresponding numerical calculations of the values with the use of experimental data obtained in [6].

Since the qualitative composition of the local structure in the case of a mix is almost impossible to establish [28], we set the value of $S_{12}(0)$ the parameter, which is determined by comparing the theoretically obtained expression with the experimental observations. In this way, using the Kirkwood-Buff formula (1), given formulas (10) and (12) obtained on the basis of the Carnahan-Starling equations, we can obtain the 12th power algebraic equation with respect to the packing parameter (η). Figure 2 presents the data of numerical solutions of this equation in comparison with the corresponding experimental data.

As can be seen from Fig. 2, we have obtained a good agreement of the theoretical approach with the data of experimental observations in the whole range of possible values of the volume fraction. It should be noted that the theoretical models involved, unlike the previous approaches, do not contain restrictions on the volume fraction of the components.

Another comment should be made in relation to the packing rate of the bi-component micromechanical mix for which the possibility of abnormal growth has been established in [6]. Given that the packing of granular substance has been described by the known logarithmic law obtained in [19], it seems that this circumstance is in accordance with the estimates for the characteristic packing time $\tau = \exp\left\{\frac{\eta_\infty}{\eta_\infty - \eta}\right\}$ (where η_∞ corresponds to the asymptotic packing), which are derived from the free volume model [29] provided that $\eta \to \eta_\infty$. However, it should be noted that the evaluation formula is set for monodisperse system, and strictly speaking, its application to granular mix requires a more substantial justification, which has not been provided so far.

The models considered use the notion of granular particles in the form of solid spheres, albeit

with different diameters, which for real systems is, of course, idealization. The influence of particle morphology on their structural agglomeration has been studied in [35]. In particular, it has been found that the granule morphology significantly affects the dynamics of compaction. The presence of anisotropic grains leads to two different compaction modes, separated by a "burst" of the packing fraction. Also, friction changes the order of placement of grains in the bulk. These observations have been confirmed by numerical simulations. The possible appearance of cohesive forces between the particles can lead to containing the compaction and reduce the values of the packing fraction.

The developed approach can be used in the case of some liquid mixes, for which the effects of packing (compaction) play a significant role [36, 4]. For example, using the Carnahan-Starling model and the data of experiments performed in [36], we can show that the dependence of excessive compaction and compressibility factors on the molar (or volume) fraction of one of the components is described by nonmonotonic laws and has extremums (Fig. 3). The established regularities have enabled applying the proposed approach to fundamentally different physical properties of systems, both micromechanical and liquid ones (with fundamentally different nature of particle interactions), in order to form their predicted properties in accordance with the needs and conditions of their use in technological processes.

Based on the analysis of experimental data on the dynamics of binary granular systems, which includes measuring their compaction and studying the impact of the ratio of component sizes and partial parameters on the compaction process, it has been concluded that it is possible to increase the degree and rate of packing, which are important factors in terms of practical application of such binary systems. In order to theoretically describe and to substantiate empirical data in the full range of values of the volume (or molar) fraction, the Kirkwood-Buff theory in combination

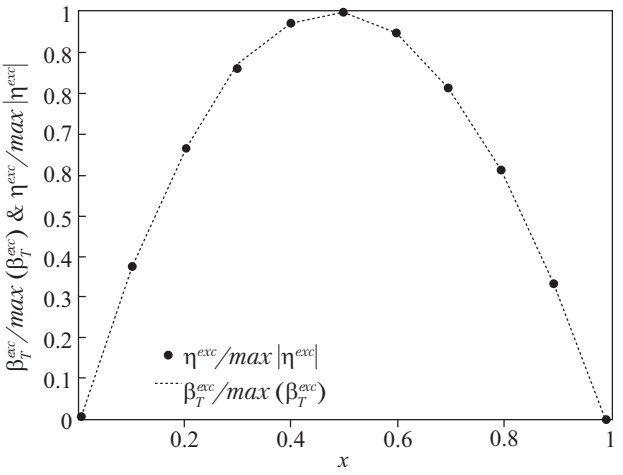

Fig. 3. Excessive compaction $\eta^{exc} = \eta - \eta^{id}$ and compressibility $\beta_T^{exc} = \beta_T - \beta_T^{id}$ factors (normalized to the corresponding values in the extremums) for the liquid mix CCl_4 + $CHCl_3$ on the molar fraction x of the second component are determined with the use of the approach developed in this research. The values of the functions η^{id} and β_T^{id}, which describe the corresponding characteristics of the so-called "ideal" states, are approximated by means of their linear approximation in the range from $x = 0$ to $x = 1$ (the so-called Raoul's law). Within the limits of the defined interval x, η^{id} and β_T^{id} describe functions η and β_T for monodisperse states (reference data) of the mix (i.e. pure components)

with the Carnahan-Starling type solid spheres models, as well as relevant phenomenological data have been used. The theoretical results coincide well with the experimental ones. The obtained data can be used to take into account the effect of multi-dispersion and to develop innovative approaches to optimizing the manipulative dynamics of compaction (compactification) of discrete micro-mechanical materials, i.e. controlling the ability of granular mix to change local structure, degree, and rate of packing, and some other parameters that are important for the practical use of the mixes in appropriate protective technologies.

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REFERENCES

1. Uchida, T., Kawahara, Y., Hayashi, Y., Tateishi, A. (2020). Eulerian Deposition Model for Sediment Mixture in Gravel-Bed Rivers with Broad Particle Size Distributions. *Journal of Hydraulic Engineering*, 146(10), 04020071. doi: 10.1061/(ASCE)HY.1943-7900.0001783.
2. Knott, J. F. (1978). *Fundamentals of fracture mechanics*. Moscow: Metallurgiya [in Russian].
3. Gerasymov, O. I., Khudyntsev, M. M., Andrianova, I. S., Spivak, A. Ya. (2016, November). Granular materials in utilization technologies of radiation-harmful substations. *Proceedings of the National Forum: "Problems, perspectives and strategy of waste utilization in Ukraine" (22–23 Nov 2016, Kyiv)*, 40–42. Kyiv [in Ukrainian].
4. Gerasymov, O. I., Somov, M. M. (2015). Statistical description of excess properties of many-particle binary systems. *Ukrainian Journal of Physics*, 60(4), 324–327. doi: 10.15407/ujpe60.04.0324.
5. Gerasymov, O. I., Zagorodny, A. G., Somov, M. M. (2013). Toward the analysis of the structure of granular materials. *Ukrainian Journal of Physics*, 58(1), 32–39. doi: 10.15407/ujpe58.01.0032.
6. Pillitteri, S., Lumay, G., Opsomer, E., Vandewalle, N. (2019). From jamming to fast compaction dynamics in granular binary mixtures. *Scientific Reports*, 9(1), 7281. doi: 10.1038/s41598-019-43519-6.
7. Jaeger, H. M., Nagel, S. R. (1992). Physics of the granular state. *Science*, 255(5051), 1523–1531. doi: 10.1126/science.255.5051.1523.
8. Aste, T., Weaire, D. (2000). *The Pursuit of Perfect Packing*. Bristol. doi: 10.1887/0750306483.
9. Weitz, D. A. (2004). Packing in the spheres. *Science*, 303(5660), 968–969. doi: 10.1126/science.1094581.
10. Torquato, S. (2018). Perspective: Basic understanding of condensed phases of matter via packing models. *The Journal of chemical physics*, 149(2), 020901. doi: 10.1063/1.5036657.
11. Torquato, S., Stillinger, F. H. (2010). Jammed hard-particle packings: From Kepler to Bernal and beyond. *Reviews of modern physics*, 82(3), 2633–2672. doi:10.1103/RevModPhys.82.2633.
12. Berryman, J. G. (1983). Random close packing of hard spheres and disks. *Physical Review A*, 27(2), 1053–1061. doi: 10.1103/PhysRevA.27.1053.
13. Onoda, G. Y., Liniger, E. G. (1990). Random loose packings of uniform spheres and the dilatancy onset. *Physical review letters*, 64(22), 2727–2730. doi: 10.1103/PhysRevLett.64.2727.
14. Song, C., Wang, P., Makse, H. A. (2008). A phase diagram for jammed matter. *Nature*, 453(7195), 629–632. doi: 10.1038/nature06981.
15. Noirhomme, M., Ludewig, F., Vandewalle, N., Opsomer, E. (2017). Cluster growth in driven granular gases. *Physical Review E*, 95(2), 022905 doi: 10.1103/PhysRevE.95.022905.
16. Lumay, G., Vandewalle, N. (2005). Experimental study of granular compaction dynamics at different scales: grain mobility, hexagonal domains, and packing fraction. *Physical review letters*, 95(2), 028002. doi: 10.1103/PhysRevLett.95.028002.
17. Carvente, O., Ruiz-Suarez, J. (2005). Crystallization of confined non-brownian spheres by vibrational annealing. *Physical review letters*, 95(1), 018001. doi: 10.1103/PhysRevLett.95.018001.
18. Panaitescu, A., Reddy, K. A., Kudrolli, A. (2012). Nucleation and crystal growth in sheared granular sphere packings. *Physical review letters*, 108(10), 108001. doi: 10.1103/PhysRevLett.108.108001.
19. Knight, J. B., Fandrich, C. G., Lau, C. N., Jaeger, H. M., Nagel, S. R. (1995). Density relaxation in a vibrated granular material. *Physical Review E*, 51(5), 3957–3963. doi:10.1103/PhysRevE.51.3957.
20. de Richter, S. K., Hanotin, C., Marchal, P., Leclerc, S., Demeurie, F., Louvet, N. (2015). Vibration-induced compaction of granular suspensions. *The European Physical Journal E*, 38(7), 74. doi: 10.1140/epje/i2015-15074-7.
21. Nicolas, M., Duru, P., Pouliquen, O. (2000). Compaction of a granular material under cyclic shear. *The European Physical Journal E*, 3(4), 309–314. doi:10.1007/s101890070001.

22. Roquier, G. (2016). The 4-parameter compressible packing model (cpm) including a new theory about wall effect and loosening effect for spheres. *Powder Technology*, 302, 247—253. doi: 10.1016/j.powtec.2016.08.031.
23. Farr, R. S., Groot, R. D. (2009). Close packing density of polydisperse hard spheres. *The Journal of chemical physics*, 131(24), 244104. doi: 10.1063/1.3276799.
24. Danisch, M., Jin, Y., Makse, H. A. (2010). Model of random packings of different size balls. *Physical Review E*, 81(5), 051303. doi:10.1103/PhysRevE.81.051303.
25. Chen, D., Torquato, S. (2015). Confined disordered strictly jammed binary sphere packings. *Physical Review E*, 92(6), 062207. doi:10.1103/PhysRevE.92.062207.
26. Hopkins, A. B., Jiao, Y., Stillinger, F. H., Torquato, S. (2011). Phase diagram and structural diversity of the densest binary sphere packings. *Physical Review Letters*, 107(12), 125501. doi:10.1103/PhysRevLett.107.125501.
27. Behringer, R. P., Chakraborty, B. (2018). The physics of jamming for granular materials: a review. *Reports on Progress in Physics*, 82(1), 012601. doi: 10.1088/1361-6633/aadc3c.
28. Boutreux, T., de Gennes, P. G. (1997). Compaction of granular mixtures: a free volume model. *Physica A*, 244(1—4), 59—67. doi: 10.1016/S0378-4371(97)00236-7.
29. Gerasymov, O. I., Khudyntsev, N. N., Klymenkov, O. A., Spivak, A. Y. (2005). The kinetics of processes occurring in granular materials in the field of vibroaccelerations. *Ukrainian Journal of Physics*, 50(6), 623—631.
30. Gerasymov, O. I., Vandewalle, N., Spivak, A. Ya., Khudyntsev, N. N., Lumay, G., Dorbolo, S., Klymenkov, O. A. (2008). Stationary states in a 1D system of inelastic particles. *Ukrainian Journal of Physics*, 53(11), 1128—1135.
31. Kirkwood, J. G., Buff, F. P. (1951). The statistical mechanical theory of solutions. I. *The Journal of chemical physics*, 19(6), 774—777. doi:10.1063/1.1748352.
32. Carnahan, N. F., Starling, K. E. (1969). Equation of state for nonattracting rigid spheres. *The Journal of chemical physics*, 51(2), 635—636. doi:10.1063/1.1672048.
33. Mansoori, G. A., Carnahan, N. F., Starling K.E., Leland Jr., T. W. (1971). Equilibrium Thermodynamic Properties of the Mixture of Hard Spheres. *The Journal of Chemical Physics*, 54(4), 1523—1525. doi:10.1063/1.1675048.
34. Pillitteri, S., Opsomer, E., Lumay, G., Vandewalle, N. (2020). How size ratio and segregation affect the packing of binary granular mixtures. *Soft Matter*, 16(39), 9094-9100. doi: 10.1039/D0SM00939C.
35. Vandewalle, N., Lumay, G., Gerasimov, O., Ludewig, F. (2007). The influence of grain shape, friction and cohesion on granular compaction dynamics. *The European Physical Journal E*, 22(3), 241—248. doi:10.1140/epje/e2007-00031-0.
36. Aliotta, F., Gapiński, J., Pochylski, M., Ponterio, R. C., Saija, F., Salvato, G. (2007). Excess compressibility in binary liquid mixtures. *The Journal of chemical physics*, 126(22), 224508. doi:10.1063/1.2745292.

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УЩІЛЬНЕННЯ (КОМПАКТИЗАЦІЯ) ВПАКУВАННЯ У БІ-КОМПОНЕНТНІЙ МІКРОМЕХАНІЧНІЙ (ГРАНУЛЬОВАНІЙ) СУМІШІ

Вступ. Одна з традиційно актуальних проблем теоретичного базису виробництва і технологій - це опис, параметризація та прогнозування властивостей суміші залежно від параметрів компонентів. Однією із найсуттєвіших проблем, які заважають ефективному використанню гранульованих матеріалів, наприклад у будівельній промисловості, є складність забезпечення їх максимального ущільнення для підвищення ефективності практичного застосування.

Проблематика. Розуміння принципів, завдяки яким формуються основні параметри багатокомпонентних систем спирається на базові моделі, які дозволяють параметризувати дані вимірів в термінах величин, що характеризують

окремі чисті компоненти (*reference data*). Побудова таких моделей є складною задачею та вимагає феноменологічної інформації із декількох альтернативних джерел.

Мета. Спираючись на апарат теорії Кірквуда-Баффа, модельні рівняння стану та данні аналізу експериментальних даних з вивчення макроскопічних параметрів бідисперсної мікромеханічної суміші побудувати теоретичний алгоритм опису та параметризації їх фізико-механічних характеристик в термінах зв'язків макроскопічних та парціальних властивостей залежно від об'ємної (або молярної) фракції одного з компонентів.

Матеріали й методи. Моделі гранульованих бікомпонентних сумішей; теорія Кірквуда-Баффа; модельні рівняння стану для модельних сумішей твердих кульок типу Карнахана-Старлінга; феноменологічна інформація про динаміку ущільнення простих гранульованих сумішей.

Результати. За допомогою теорії Кірквуда-Баффа, модельних співвідношень для сумішей твердих кульок, із використанням феноменологічних даних про характер ущільнення гранульованих матеріалів, розроблено алгоритм для опису макроскопічних властивостей бінарних гранульованих систем зокрема компактизації.

Висновки. Отримані дані підтверджують наявність впливу мультидисперсності на динаміку ущільнення тобто, на можливість суміші під дією зовнішніх впливів прогнозовано змінювати локальну структуру впакування та її параметри.

Ключові слова: захисні гранульовані екрани, гранульована бікомпонентна суміш, теорія Кірквуда-Баффа, впакування, ущільнення, модель Карнахана-Старлінга, рідинні суміші, надлишкові властивості сумішів.